Electronic Supplementary Material (ESI) for CrystEngComm.

A One Dimensional Coordination Polymer Composed of Antiferromagnetically Coupled Disk-like [Mn_7] Units

Supporting Information

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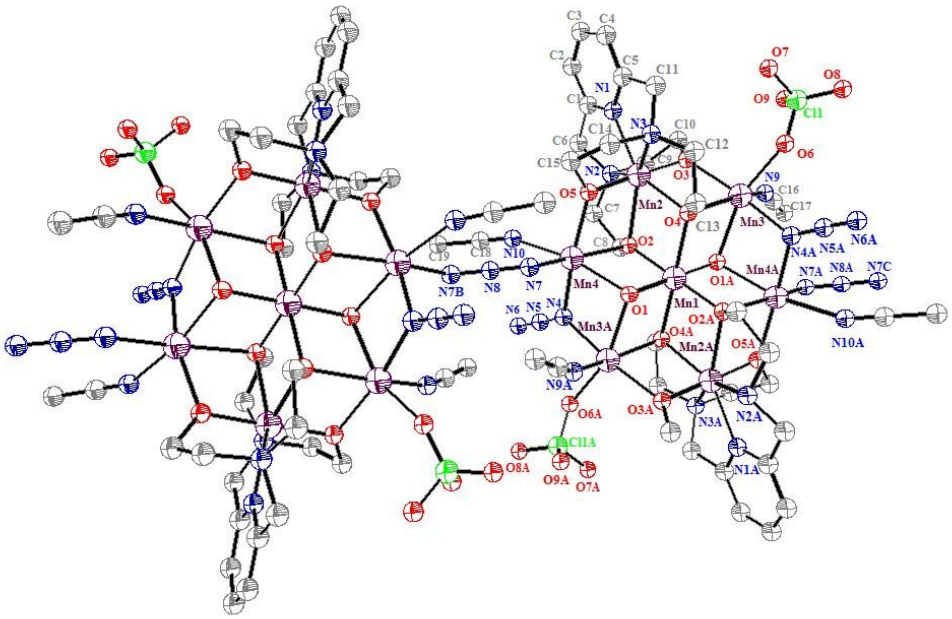


Table 1S. BVS Calculation of compound **1**

Atom	Mn^{II}	Mn^{III}	Mn^{IV}
Mn(1)	3.035797	**2.77676**	2.915185
Mn(2)	3.12313	**2.912701**	2.966887
Mn(3)	**2.094367**	1.960452	1.985461
Mn(4)	**2.105679**	1.987834	2.358428

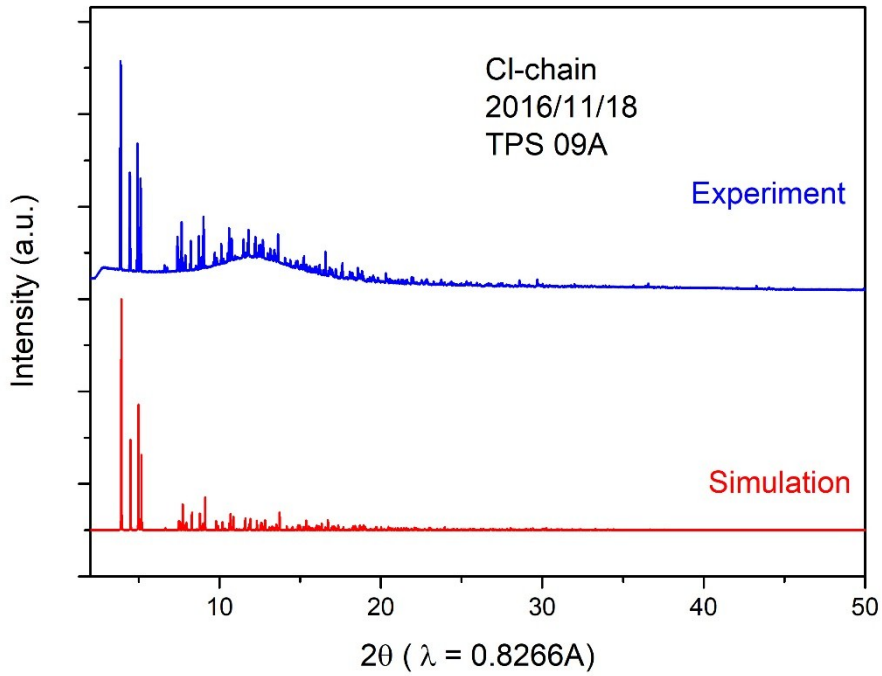


Figure 2S. Powder X-ray diffraction data for compound 1 with 2θ up to 50°.

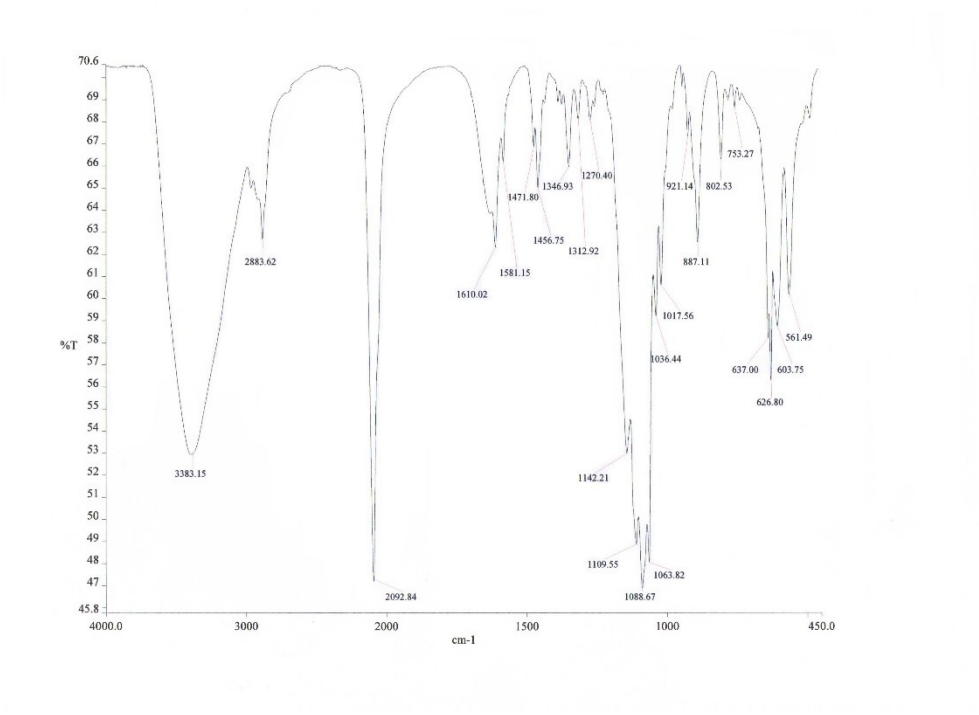


Figure 3S. IR spectra of compound **1**.

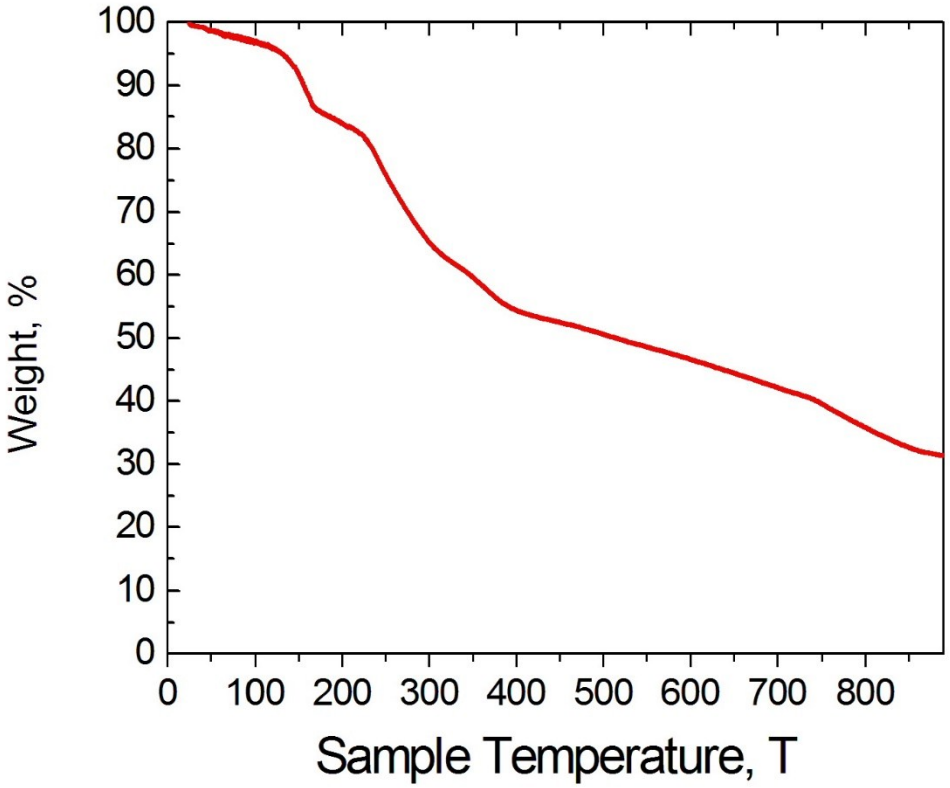
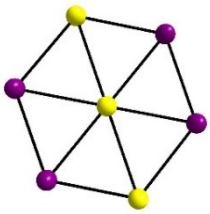
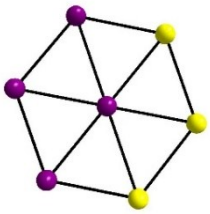
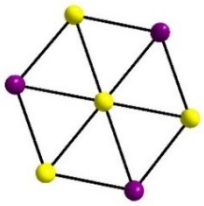
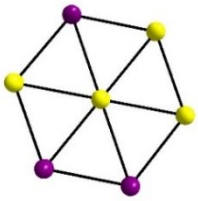
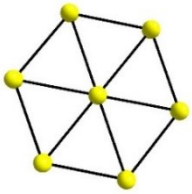
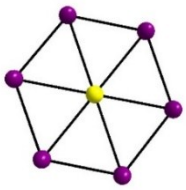
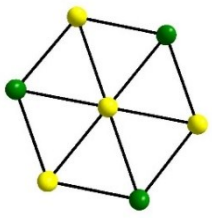
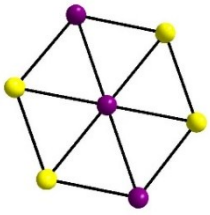


Figure 4S. TGA plot of compound **1**.

Table 2S Comparison of disk like Mn7 complexes.

(a) 	(b) 
$[Mn^{II}_3Mn^{III}_4(OMe)_{12}(dbm)_6]\cdot CHCl_3\cdot 14MeOH$ $[Mn^{II}_3Mn^{III}_4(5\text{-}NO_2\text{-}hbide)_6]\cdot 5C_2H_4Cl_2$ $\{Mn^{II}[Mn^{II}_2Mn^{III}_4Cl_6(L^3)_6]\}\cdot 2CHCl_3$	$[Mn^{II}_3Mn^{III}_4(nmdea)_6(N_3)_6]\cdot CH_3OH$
(c) 	(d) 
$[Mn^{II}_4Mn^{III}_3(OH)_3(hmp)_9Cl_3](Cl)(ClO_4)$ $[Mn^{II}_4Mn^{III}_3(teaH)_3(tea)_3](ClO_4)_2\cdot 3MeOH$ $[NEt_4]\{Mn^{II}[Mn^{II}_3Mn^{III}_3Cl_6(mda)_6]\}$ $\{[Na(MeOH)_3][Mn^{II}_4Mn^{III}_3(N_3)_6(mda)_6]\}_n$ $(NHEt_3)[Mn^{II}_4Mn^{III}_3Cl_6(mda)_6]$ $(NHEt_3)[Mn^{II}_4Mn^{III}_3(N_3)_6(mda)_6]$ $\{Na[Mn^{II}_4Mn^{III}_3(N_3)_6(teaH)_6]\}_n$ $(NHEt_3)[Mn^{II}_4Mn^{III}_3(N_3)_6(teaH)_6]$	$[Mn^{II}_4Mn^{III}_3F_3(tea)(teaH)(teaH_2)_2(piv)_4(Hpiv)(chp)_3]\cdot 0.5MeCN$
(e) 	(f) 
$[Mn^{II}_7(pppd)_6(tea)(OH)_3][BF_4]_2\cdot 2MeOH\cdot 2CH_2Cl_2$ $[Mn^{II}_7(paa)_6(OMe)_6][NO_3]_2\cdot 6MeOH$	$[Mn^{II}Mn^{III}_6(heamp)_6](ClO_4)_2\cdot 4CH_2Cl_2\cdot H_2O$
(g) 	(h) 
$[Mn^{II}_4Mn^{IV}_3(tea)(teaH_2)_3(peolH)_4]($	{[

$BF_4)_2 \cdot solv$	$Mn^{II}_4Mn^{III}_3(OH)_2(dhap)_2(N_3)_3(MeCN)_4(ClO_4)_2] \cdot 2($ $MeCN) \cdot 2(ClO_4)\}_\infty$

Table 3S. Crystal data and structure refinement for **1**.

Identification code	**1**	
Empirical formula	C42 H64 Cl4 Mn7 N21 O26	
Formula weight	1805.52	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 20.8441(10) Å	α= 90°.
	b = 16.0569(8) Å	β= 114.1605(11)°.
	c = 23.1343(11) Å	γ = 90°.
Volume	7064.6(6) $Å^3$	
Z	4	
Density (calculated)	1.698 Mg/m^3	
Absorption coefficient	1.451 mm^{-1}	
F(000)	3656	
Crystal size	0.32 x 0.25 x 0.25 mm^3	
Theta range for data collection	1.66 to 27.50°.	
Index ranges	-27<=h<=25, -20<=k<=20, -29<=l<=30	
Reflections collected	26970	
Independent reflections	8104 [R(int) = 0.0392]	
Completeness to theta = 27.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7130 and 0.6538	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8104 / 134 / 472	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0527, wR2 = 0.1438	
R indices (all data)	R1 = 0.0664, wR2 = 0.1529	
Largest diff. peak and hole	0.934 and -0.731 e.$Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

x	y	z	U(eq)	
Mn(1)	2500	7500	0	19(1)
Mn(2)	2223(1)	5442(1)	-360(1)	27(1)
Mn(3)	3186(1)	6024(1)	1082(1)	28(1)
Mn(4)	3532(1)	8056(1)	1438(1)	27(1)
Cl(1)	3153(3)	4424(4)	1997(3)	58(1)
Cl(1')	2944(4)	4530(5)	2059(4)	58(1)
O(1)	3420(1)	7215(2)	645(1)	23(1)
O(2)	2549(1)	6724(2)	-636(1)	26(1)
O(3)	3028(1)	5157(2)	354(1)	33(1)
O(4)	2168(1)	6342(2)	302(1)	27(1)
O(5)	1422(1)	5755(2)	-1077(1)	33(1)
O(6)	2998(4)	5232(4)	1764(3)	65(1)
O(7)	2580(6)	3874(6)	1629(5)	80(2)
O(8)	3282(7)	4374(10)	2622(5)	127(3)
O(9)	3783(6)	4185(6)	1889(6)	112(2)
O(6')	3019(6)	4816(5)	1500(4)	65(1)
O(7')	2734(8)	3716(7)	1980(6)	80(2)
O(8')	3662(9)	4444(14)	2590(7)	127(3)
O(9')	2475(8)	5037(7)	2176(7)	112(2)
N(1)	2060(2)	4131(2)	-638(2)	32(1)
N(2)	2976(2)	5140(2)	-834(2)	32(1)
N(3)	1333(2)	4942(2)	-90(2)	32(1)
N(4)	3096(2)	6959(2)	1711(1)	36(1)
N(5)	2897(2)	6928(2)	2132(2)	40(1)
N(6)	2721(3)	6915(3)	2533(2)	66(1)
N(7)	4659(2)	7865(2)	1948(2)	40(1)
N(8)	5000	7871(3)	2500	31(1)
N(9)	4329(2)	5862(2)	1494(2)	41(1)
N(10)	3581(2)	8620(2)	2340(2)	45(1)
C(1)	2326(2)	3818(2)	-1030(2)	35(1)
C(2)	2236(3)	2993(3)	-1214(2)	44(1)
C(3)	1849(3)	2492(3)	-991(2)	49(1)

C(4)	1571(3)	2814(3)	-593(2)	44(1)
C(5)	1692(2)	3640(2)	-421(2)	34(1)
C(6)	2688(2)	4440(2)	-1280(2)	42(1)
C(7)	3074(2)	5876(2)	-1176(2)	32(1)
C(8)	3136(2)	6662(2)	-804(2)	31(1)
C(9)	3652(2)	4925(3)	-294(2)	40(1)
C(10)	3518(2)	4607(2)	260(2)	36(1)
C(11)	1446(2)	4042(2)	43(2)	38(1)
C(12)	1364(2)	5405(2)	471(2)	34(1)
C(13)	1545(2)	6301(2)	419(2)	33(1)
C(14)	672(2)	5128(3)	-647(2)	40(1)
C(15)	812(2)	5245(3)	-1239(2)	38(1)
C(16)	4910(2)	5968(3)	1641(2)	46(1)
C(17)	5665(3)	6138(5)	1838(3)	72(2)
C(18)	3746(2)	8664(3)	2867(2)	42(1)
C(19)	3976(3)	8702(4)	3552(2)	66(2)
Cl(2)	119(1)	2157(1)	112(1)	40(1)
O(10)	-259(2)	2115(3)	501(2)	72(1)
O(11)	-36(2)	2922(3)	-222(2)	84(2)
O(12)	856(2)	2097(2)	488(2)	53(1)
O(13)	-102(2)	1508(3)	-341(2)	94(2)
N(11)	5824(7)	796(8)	1873(8)	219(6)
C(20)	5836(7)	1471(8)	1930(6)	149(5)
C(21)	5817(7)	2337(7)	1958(5)	159(4)

Bond lengths [Å] and angles [°] for **1**.

Mn(1)-O(1)	1.942(2)	O(2)-Mn(4)#1	2.285(2)
Mn(1)-O(1)#1	1.942(2)	O(3)-C(10)	1.434(4)
Mn(1)-O(2)#1	1.963(2)	O(4)-C(13)	1.430(4)
Mn(1)-O(2)	1.963(2)	O(5)-C(15)	1.427(4)
Mn(1)-O(4)	2.197(2)	O(5)-Mn(4)#1	2.101(3)
Mn(1)-O(4)#1	2.197(2)	N(1)-C(5)	1.333(5)
Mn(2)-O(3)	1.867(3)	N(1)-C(1)	1.342(5)
Mn(2)-O(5)	1.876(3)	N(2)-C(6)	1.477(5)
Mn(2)-O(4)	2.143(2)	N(2)-C(7)	1.484(5)
Mn(2)-N(1)	2.187(3)	N(2)-C(9)	1.491(5)
Mn(2)-N(2)	2.303(3)	N(3)-C(12)	1.471(5)
Mn(2)-N(3)	2.330(3)	N(3)-C(11)	1.476(5)
Mn(2)-O(2)	2.337(2)	N(3)-C(14)	1.481(5)
Mn(3)-O(3)	2.103(3)	N(4)-N(5)	1.204(4)
Mn(3)-N(4)	2.154(3)	N(5)-N(6)	1.130(5)
Mn(3)-O(6)	2.185(6)	N(7)-N(8)	1.181(3)
Mn(3)-N(9)	2.188(3)	N(8)-N(7)#2	1.181(3)
Mn(3)-O(4)	2.210(2)	N(9)-C(16)	1.129(6)
Mn(3)-O(6')	2.257(8)	N(10)-C(18)	1.126(5)
Mn(3)-O(1)	2.305(2)	C(1)-C(2)	1.379(5)
Mn(4)-O(5)#1	2.101(3)	C(1)-C(6)	1.502(5)
Mn(4)-N(7)	2.176(3)	C(2)-C(3)	1.380(6)
Mn(4)-N(4)	2.192(3)	C(3)-C(4)	1.373(6)
Mn(4)-O(1)	2.211(2)	C(4)-C(5)	1.378(5)
Mn(4)-N(10)	2.239(3)	C(5)-C(11)	1.512(5)
Mn(4)-O(2)#1	2.285(2)	C(7)-C(8)	1.502(5)
Cl(1)-O(8)	1.362(13)	C(9)-C(10)	1.508(6)
Cl(1)-O(6)	1.390(9)	C(12)-C(13)	1.505(5)
Cl(1)-O(7)	1.450(12)	C(14)-C(15)	1.524(6)
Cl(1)-O(9)	1.483(11)	C(16)-C(17)	1.474(7)
Cl(1')-O(7')	1.367(14)	C(18)-C(19)	1.456(6)
Cl(1')-O(9')	1.381(13)	Cl(2)-O(13)	1.415(4)
Cl(1')-O(6')	1.441(11)	Cl(2)-O(11)	1.417(4)
Cl(1')-O(8')	1.505(19)	Cl(2)-O(10)	1.418(3)
O(2)-C(8)	1.431(4)	Cl(2)-O(12)	1.426(3)

N(11)-C(20)	1.091(14)	C(20)-C(21)	1.393(15)

O(1)-Mn(1)-O(1)#1	179.998(1)	N(3)-Mn(2)-O(2)	136.87(10)
O(1)-Mn(1)-O(2)#1	84.93(10)	O(3)-Mn(3)-N(4)	166.92(12)
O(1)#1-Mn(1)-O(2)#1	95.07(10)	O(3)-Mn(3)-O(6)	100.2(2)
O(1)-Mn(1)-O(2)	95.07(10)	N(4)-Mn(3)-O(6)	79.9(2)
O(1)#1-Mn(1)-O(2)	84.93(10)	O(3)-Mn(3)-N(9)	93.29(12)
O(2)#1-Mn(1)-O(2)	180.0	N(4)-Mn(3)-N(9)	99.72(13)
O(1)-Mn(1)-O(4)	84.02(9)	O(6)-Mn(3)-N(9)	95.8(2)
O(1)#1-Mn(1)-O(4)	95.98(9)	O(3)-Mn(3)-O(4)	73.50(9)
O(2)#1-Mn(1)-O(4)	100.29(9)	N(4)-Mn(3)-O(4)	93.99(11)
O(2)-Mn(1)-O(4)	79.71(9)	O(6)-Mn(3)-O(4)	109.1(2)
O(1)-Mn(1)-O(4)#1	95.98(9)	N(9)-Mn(3)-O(4)	153.34(12)
O(1)#1-Mn(1)-O(4)#1	84.02(9)	O(3)-Mn(3)-O(6')	76.9(2)
O(2)#1-Mn(1)-O(4)#1	79.71(9)	N(4)-Mn(3)-O(6')	103.7(2)
O(2)-Mn(1)-O(4)#1	100.29(9)	O(6)-Mn(3)-O(6')	23.8(2)
O(4)-Mn(1)-O(4)#1	180.0	N(9)-Mn(3)-O(6')	92.4(3)
O(3)-Mn(2)-O(5)	178.64(12)	O(4)-Mn(3)-O(6')	106.4(3)
O(3)-Mn(2)-O(4)	79.87(10)	O(3)-Mn(3)-O(1)	101.00(10)
O(5)-Mn(2)-O(4)	99.38(11)	N(4)-Mn(3)-O(1)	79.08(10)
O(3)-Mn(2)-N(1)	89.95(12)	O(6)-Mn(3)-O(1)	158.72(19)
O(5)-Mn(2)-N(1)	91.32(12)	N(9)-Mn(3)-O(1)	84.40(11)
O(4)-Mn(2)-N(1)	144.23(11)	O(4)-Mn(3)-O(1)	75.85(9)
O(3)-Mn(2)-N(2)	80.14(12)	O(6')-Mn(3)-O(1)	176.1(3)
O(5)-Mn(2)-N(2)	99.74(12)	O(5)#1-Mn(4)-N(7)	97.39(12)
O(4)-Mn(2)-N(2)	136.76(10)	O(5)#1-Mn(4)-N(4)	159.54(12)
N(1)-Mn(2)-N(2)	73.25(11)	N(7)-Mn(4)-N(4)	102.32(14)
O(3)-Mn(2)-N(3)	101.74(12)	O(5)#1-Mn(4)-O(1)	103.44(10)
O(5)-Mn(2)-N(3)	79.13(11)	N(7)-Mn(4)-O(1)	95.06(11)
O(4)-Mn(2)-N(3)	76.02(10)	N(4)-Mn(4)-O(1)	80.36(10)
N(1)-Mn(2)-N(3)	72.65(11)	O(5)#1-Mn(4)-N(10)	90.65(13)
N(2)-Mn(2)-N(3)	145.84(11)	N(7)-Mn(4)-N(10)	85.62(13)
O(3)-Mn(2)-O(2)	101.61(10)	N(4)-Mn(4)-N(10)	85.49(13)
O(5)-Mn(2)-O(2)	77.07(10)	O(1)-Mn(4)-N(10)	165.65(12)
O(4)-Mn(2)-O(2)	73.07(9)	O(5)#1-Mn(4)-O(2)#1	74.19(9)
N(1)-Mn(2)-O(2)	142.68(10)	N(7)-Mn(4)-O(2)#1	161.65(11)
N(2)-Mn(2)-O(2)	74.00(10)	N(4)-Mn(4)-O(2)#1	88.33(11)

O(1)-Mn(4)-O(2)#1	71.77(9)	C(5)-N(1)-C(1)	119.6(3)
N(10)-Mn(4)-O(2)#1	110.36(12)	C(5)-N(1)-Mn(2)	120.2(2)
O(8)-Cl(1)-O(6)	112.3(9)	C(1)-N(1)-Mn(2)	120.2(2)
O(8)-Cl(1)-O(7)	110.1(8)	C(6)-N(2)-C(7)	109.8(3)
O(6)-Cl(1)-O(7)	109.7(7)	C(6)-N(2)-C(9)	112.5(3)
O(8)-Cl(1)-O(9)	111.0(9)	C(7)-N(2)-C(9)	110.0(3)
O(6)-Cl(1)-O(9)	105.1(6)	C(6)-N(2)-Mn(2)	109.4(2)
O(7)-Cl(1)-O(9)	108.5(7)	C(7)-N(2)-Mn(2)	110.9(2)
O(7')-Cl(1')-O(9')	112.1(10)	C(9)-N(2)-Mn(2)	104.2(2)
O(7')-Cl(1')-O(6')	109.4(8)	C(12)-N(3)-C(11)	111.4(3)
O(9')-Cl(1')-O(6')	109.5(9)	C(12)-N(3)-C(14)	110.9(3)
O(7')-Cl(1')-O(8')	100.2(11)	C(11)-N(3)-C(14)	113.0(3)
O(9')-Cl(1')-O(8')	116.2(11)	C(12)-N(3)-Mn(2)	108.0(2)
O(6')-Cl(1')-O(8')	109.0(9)	C(11)-N(3)-Mn(2)	108.4(2)
Mn(1)-O(1)-Mn(4)	103.26(10)	C(14)-N(3)-Mn(2)	104.8(2)
Mn(1)-O(1)-Mn(3)	102.35(10)	N(5)-N(4)-Mn(3)	132.3(3)
Mn(4)-O(1)-Mn(3)	96.54(9)	N(5)-N(4)-Mn(4)	125.9(3)
C(8)-O(2)-Mn(1)	124.1(2)	Mn(3)-N(4)-Mn(4)	101.72(12)
C(8)-O(2)-Mn(4)#1	117.3(2)	N(6)-N(5)-N(4)	178.4(5)
Mn(1)-O(2)-Mn(4)#1	99.98(10)	N(8)-N(7)-Mn(4)	128.7(2)
C(8)-O(2)-Mn(2)	113.0(2)	N(7)-N(8)-N(7)#2	179.2(6)
Mn(1)-O(2)-Mn(2)	104.11(10)	C(16)-N(9)-Mn(3)	162.9(4)
Mn(4)#1-O(2)-Mn(2)	93.26(9)	C(18)-N(10)-Mn(4)	155.9(4)
C(10)-O(3)-Mn(2)	117.1(2)	N(1)-C(1)-C(2)	121.8(4)
C(10)-O(3)-Mn(3)	129.8(2)	N(1)-C(1)-C(6)	115.0(3)
Mn(2)-O(3)-Mn(3)	109.64(12)	C(2)-C(1)-C(6)	123.1(4)
C(13)-O(4)-Mn(2)	114.9(2)	C(1)-C(2)-C(3)	118.2(4)
C(13)-O(4)-Mn(1)	121.8(2)	C(4)-C(3)-C(2)	120.1(4)
Mn(2)-O(4)-Mn(1)	103.09(10)	C(3)-C(4)-C(5)	118.7(4)
C(13)-O(4)-Mn(3)	118.6(2)	N(1)-C(5)-C(4)	121.7(4)
Mn(2)-O(4)-Mn(3)	96.49(9)	N(1)-C(5)-C(11)	115.4(3)
Mn(1)-O(4)-Mn(3)	97.62(9)	C(4)-C(5)-C(11)	122.9(3)
C(15)-O(5)-Mn(2)	117.0(2)	N(2)-C(6)-C(1)	111.2(3)
C(15)-O(5)-Mn(4)#1	126.7(2)	N(2)-C(7)-C(8)	111.2(3)
Mn(2)-O(5)-Mn(4)#1	115.18(12)	O(2)-C(8)-C(7)	109.3(3)
Cl(1)-O(6)-Mn(3)	137.7(5)	N(2)-C(9)-C(10)	110.4(3)
Cl(1')-O(6')-Mn(3)	138.7(6)	O(3)-C(10)-C(9)	108.2(3)

N(3)-C(11)-C(5)	110.0(3)
N(3)-C(12)-C(13)	109.6(3)
O(4)-C(13)-C(12)	109.6(3)
N(3)-C(14)-C(15)	110.9(3)
O(5)-C(15)-C(14)	108.1(3)
N(9)-C(16)-C(17)	177.9(6)
N(10)-C(18)-C(19)	178.3(5)
O(13)-Cl(2)-O(11)	107.5(3)
O(13)-Cl(2)-O(10)	109.7(3)
O(11)-Cl(2)-O(10)	109.0(3)
O(13)-Cl(2)-O(12)	110.2(2)
O(11)-Cl(2)-O(12)	109.8(2)
O(10)-Cl(2)-O(12)	110.5(2)
N(11)-C(20)-C(21)	175.9(17)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+3/2,-z #2 -x+1,y,-z+1/2

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}	
Mn(1)	17(1)	25(1)	16(1)	1(1)	7(1)	1(1)
Mn(2)	22(1)	26(1)	33(1)	-3(1)	11(1)	-2(1)
Mn(3)	26(1)	34(1)	22(1)	5(1)	9(1)	3(1)
Mn(4)	25(1)	37(1)	18(1)	0(1)	6(1)	-1(1)
Cl(1)	89(3)	41(2)	44(1)	2(1)	27(2)	-11(2)
Cl(1')	89(3)	41(2)	44(1)	2(1)	27(2)	-11(2)
O(1)	20(1)	29(1)	19(1)	2(1)	8(1)	1(1)
O(2)	20(1)	32(1)	29(1)	2(1)	12(1)	0(1)
O(3)	29(1)	31(1)	37(1)	-3(1)	12(1)	5(1)
O(4)	21(1)	37(1)	25(1)	-1(1)	13(1)	0(1)
O(5)	25(1)	37(1)	34(1)	0(1)	10(1)	-8(1)
O(6)	110(4)	47(3)	51(3)	4(2)	46(3)	-7(3)
O(7)	105(5)	45(3)	98(6)	-9(4)	51(6)	-16(4)
O(8)	123(7)	192(8)	50(3)	22(4)	21(4)	-32(7)
O(9)	146(6)	71(4)	158(7)	-9(4)	104(6)	0(4)
O(6')	110(4)	47(3)	51(3)	4(2)	46(3)	-7(3)
O(7')	105(5)	45(3)	98(6)	-9(4)	51(6)	-16(4)
O(8')	123(7)	192(8)	50(3)	22(4)	21(4)	-32(7)
O(9')	146(6)	71(4)	158(7)	-9(4)	104(6)	0(4)
N(1)	35(2)	34(2)	32(2)	-5(1)	18(1)	-6(1)
N(2)	33(2)	27(2)	42(2)	1(1)	21(2)	-2(1)
N(3)	30(2)	35(2)	34(2)	-4(1)	15(1)	-4(1)
N(4)	38(2)	50(2)	22(2)	4(1)	16(1)	1(2)
N(5)	49(2)	42(2)	37(2)	5(2)	26(2)	5(2)
N(6)	106(4)	60(3)	66(3)	4(2)	69(3)	3(3)
N(7)	26(2)	59(2)	27(2)	-4(2)	2(1)	1(2)
N(8)	24(2)	32(2)	34(3)	0	10(2)	0
N(9)	28(2)	45(2)	44(2)	5(2)	8(2)	4(2)
N(10)	45(2)	60(2)	27(2)	-9(2)	13(2)	-1(2)
C(1)	44(2)	29(2)	39(2)	-4(2)	24(2)	-7(2)
C(2)	58(3)	36(2)	50(3)	-7(2)	35(2)	-6(2)
C(3)	74(3)	27(2)	57(3)	-9(2)	39(3)	-13(2)
C(4)	60(3)	33(2)	51(3)	-4(2)	37(2)	-11(2)

C(5)	39(2)	32(2)	35(2)	-3(2)	19(2)	-7(2)
C(6)	56(3)	34(2)	52(3)	-10(2)	39(2)	-12(2)
C(7)	32(2)	31(2)	41(2)	1(2)	21(2)	-2(2)
C(8)	27(2)	31(2)	41(2)	2(2)	21(2)	-1(1)
C(9)	32(2)	37(2)	56(3)	7(2)	22(2)	10(2)
C(10)	34(2)	31(2)	44(2)	2(2)	16(2)	8(2)
C(11)	46(2)	35(2)	42(2)	-2(2)	27(2)	-7(2)
C(12)	32(2)	39(2)	37(2)	-6(2)	22(2)	-3(2)
C(13)	29(2)	39(2)	40(2)	-4(2)	22(2)	1(2)
C(14)	26(2)	55(3)	40(2)	-2(2)	12(2)	-7(2)
C(15)	28(2)	45(2)	37(2)	-3(2)	8(2)	-12(2)
C(16)	40(2)	60(3)	33(2)	7(2)	10(2)	9(2)
C(17)	36(3)	117(5)	58(3)	5(3)	14(2)	2(3)
C(18)	41(2)	46(2)	39(2)	-6(2)	17(2)	-3(2)
C(19)	67(3)	96(4)	31(2)	-8(3)	17(2)	-3(3)
Cl(2)	26(1)	48(1)	52(1)	2(1)	20(1)	0(1)
O(10)	31(2)	142(4)	50(2)	27(2)	23(2)	12(2)
O(11)	49(2)	89(3)	123(4)	55(3)	43(2)	21(2)
O(12)	25(2)	62(2)	73(2)	3(2)	19(2)	6(1)
O(13)	59(3)	104(4)	111(4)	-52(3)	25(3)	-6(2)
N(11)	169(11)	149(10)	288(17)	-23(11)	44(11)	-60(9)
C(20)	142(10)	126(9)	156(10)	-56(8)	37(8)	-51(8)
C(21)	186(9)	146(8)	129(7)	-9(6)	47(6)	-11(7)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1**.

x	y	z	U(eq)	
H(2)	2436	2777	-1485	52
H(3)	1774	1923	-1114	59
H(4)	1301	2475	-440	52
H(6A)	3075	4161	-1349	50
H(6B)	2349	4656	-1693	50
H(7A)	2669	5924	-1593	38
H(7B)	3504	5802	-1253	38
H(8A)	3580	6654	-417	37
H(8B)	3146	7150	-1062	37
H(9A)	3956	5425	-165	48
H(9B)	3900	4493	-430	48
H(10A)	3324	4036	173	43
H(10B)	3964	4592	645	43
H(11A)	1002	3779	8	46
H(11B)	1803	3958	481	46
H(12A)	1725	5155	859	40
H(12B)	904	5372	500	40
H(13A)	1151	6574	68	40
H(13B)	1623	6598	816	40
H(14A)	458	5641	-567	49
H(14B)	335	4665	-715	49
H(15A)	890	4698	-1397	46
H(15B)	403	5515	-1577	46
H(17A)	5722	6646	1628	108
H(17B)	5884	5668	1717	108
H(17C)	5889	6214	2298	108
H(19A)	4430	8419	3759	99
H(19B)	3627	8429	3670	99
H(19C)	4026	9286	3687	99
H(21A)	5673	2568	1531	239
H(21B)	6284	2547	2231	239
H(21C)	5478	2506	2131	239